Fossil Energy Research Grants Awarded to Four Minority Universities Students, Faculty to Collaborate in

Students, Faculty to Collaborate in Innovative Projects

Washington, DC—Continuing its long-standing minority university research program, the Department of Energy has selected four institutions where students and faculty will investigate projects dealing with sensors and controls, computational energy sciences, and advanced materials for use in fossil fuel power systems.

The universities were chosen as the winners in DOE's annual competition for fossil energy research ideas from the nation's Historically Black Colleges and Universities and Other Minority Institutions (HBCU/OMI).

"I am pleased to announce the selection of four outstanding projects that will afford students and their professors the opportunity to tackle highly relevant fossil energy issues," said James A. Slutz, acting Assistant Secretary for Fossil Energy. "Their curiosity and tenacity as learners will serve these students well as they help promote our nation's energy security and assure the growth of future energy researchers."

Established in 1984, the HBCU/OMI program was designed to encourage cooperative fossil energy research and development projects between HBCU/OMI, U.S. industries, and federal agencies. The program is carried out under DOE's Office of Fossil Energy and gives minority students valuable hands-on experience in developing technologies to promote the efficient and environmentally safe use of coal, oil, and natural gas.

Fossil Energy's National Energy Technology Laboratory (NETL) issued the funding opportunity announcement in April 2008, opening a new year of collaborative efforts between faculty-student teams and the commercial sector to develop and execute innovative research ideas. In addition to the two grants offered to study novel sensors for high-temperature fossil energy applications and multiphase flow research, a grant was awarded in each of two advanced materials subtopic areas: computer-aided development of materials and novel new materials for energy conversion.

The following universities and projects were selected:

• University of Texas, El Paso (El Paso, Texas) — Reliable, fast, highly sensitive, and selective sensors which can withstand high-temperature and chemically corrosive environments are needed for detecting and monitoring even very low concentrations of hydrogen sulfide (H2S) emissions from coal gasification power systems. This project will

focus on the development of sensors based on pure and doped tungsten oxide (WO3) for on-line monitoring and detection of H2S in the corrosive atmosphere of coal gasification systems operating at temperatures of 500ŰC or above. The researchers will assess the atomic/chemical structure, surface/interface microstructure, stability, electronic structure, and sensor performance of pure and titanium-, gold-, and aluminum-doped WO3 thin-film nanostructures for their utilization in sensor devices to effectively monitor and detect H2S. (DOE share: \$199,546; length of contract: 36 months)

- University of Texas, San Antonio (San Antonio, Texas) Gas-solids flow is prevalent in fossil fuel processes such as coal gasifiers, and the ability to understand and model these gas-solids systems is crucial for building highly efficient, near-zero emission fossil energy plants. This project is directed at improving the performance and accuracy of the Multiphase Flow with Interphase eXchanges (MFIX) code that is frequently used in multiphase flow simulations. MFIX is a general-purpose computer code developed at NETL for describing the hydrodynamics, heat transfer and chemical reactions in fluid-solids systems. MFIX calculations give transient data on the three-dimensional distribution of pressure, velocity, temperature, and species mass fractions. This research includes use of first principles embedded in a validated Direct Numerical Simulation (DNS) particulate flow program that uses the Immersed Boundary method (IB) to establish, modify and validate needed energy and boundary conditions for the MFIX code. (DOE share: \$199,884; length of contract: 24 months)
- Tennessee State University (Nashville, Tenn.)—Novel materials that can withstand high temperatures and extreme environments are crucial for the development of materials for efficient energy systems. Boron carbide has great applications in the energy industry for its many unusual properties such as low density, high mechanical strength, high melting temperature, high chemical inertness, and a propensity for high-efficiency, direct thermoelectric conversion. The crystal structure of boron carbide is rather unique and the controversy over the disordered carbon distribution in the crystal structure of boron carbides remains unsolved. This project will involve the use of large supercell models of the 15-atom crystal structure of boron carbide, allowing for a greater configuration variation of carbon, thus permitting a better understanding of the structure-properties relations. This investigation will study the electronic structure and bonding using X-ray Absorption Near Edge Spectroscopy (XANES) and Energy Loss Near Edge Spectroscopy (ELNES) methods for searching possible new phases in the configuration space of supercells, which will be carefully categorized based on lattice symmetry. It is anticipated that the result of this investigation will break new ground for boron carbide research and bring more conclusive answers to the long-lasting controversy over structure-property relationships.

(DOE share: \$186,763; length of contract: 24 months)

• North Carolina A&T State University (Greensboro, N.C.) — Steam reforming of methanol (SRM) is potentially more cost effective than the reforming of hydrocarbons for the production of high-purity hydrogen. This project proposes to investigate steam reforming of methanol with more stable catalysts and minimal production of carbon monoxide (CO). This investigation would involve the synthesis of novel palladium-cobalt (Pd-Co) and palladium-nickel (Pd-Ni) bimetallic nanocatalysts in mesoporous silica using hydrothermal and co-condensation routes in the presence of a surfactant as a structure-directing agent. Bimetallic nanocatalysts in mesoporous silica, synthesized by

the proposed novel in-situ procedure, have tremendous potential in steam reforming of methanol for hydrogen (H2) production and can have a significant impact on the H2-economy using coal-derived fuels. (DOE share: \$200,000; length of contract: 36 months)